

# **Quantum Monte Carlo Study of Weakly Interacting Systems**

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Fixed node diffusion Monte Carlo (DMC) and variational Monte Carlo (VMC) energies are calculated for two systems, water dimer and nitric oxide dimer, as examples of two different weak interaction energies. Using single determinant trial wave functions, comparison with experiments results with other levels of theory show good agreement in the preliminary results. This results important since QMC can be applicable to systems containing a large number of atoms and still get good values of this very small energies. The main result observed are result of the fixed node approximation and also the small number of blocks calculated at this time.

Weak interactions dominate most biochemical interactions. Small energy differences have been difficult to determine accurately for large systems with available quantum chemical methods. In this project we investigated the applicability of quantum Monte Carlo to the determination of interaction energies of small, but very important systems. Two types of weak interactions were studied, hydrogen-bonding, represented by the water molecule and Van der Waals interactions, which were studied in the Nitric Oxide dimmer. Calculations were made using the QMC method and different tests were made using different trial wave functions, obtained at different levels of theory and different basis set quality.

ves to be a considerable challenge for theoretical ab



 $\frac{d\phi}{dx} = -\frac{i}{d\phi} \phi_0$ 

- expectation values for a given trial wavefunction.
  Diffusion Monte Carlo (DMC) is based in the fact that the Schroedinger
  equation withten in imaginary time will converge to the ground state
  exponentially fast. (This is also known as projector Monte Carlo or Green's

ethod		H/O-H/O(seasone)	1	Method	Energy(kcal/mol)	alsNO-NO(kasi/mai)
CISD	SDVq-00-gust	-4.83 (-4.66)		CASPT2(18,14)	200.406569	4.31
FTBLYP	SDVq-10-gus	-4.19 (-4.16)		CASPT2(18,14)/ 60-977Z	218.663724	434
FTROLYP	Aug-oc-pVQZ	-4.97 (-4.94)		CASPT2(18,14)/ 869-00-07/TZ	388 SCF708	6.31
FT/RPW91	aug-oc-pVQZ	-3.88 (-3.84)		MRC(10)+Q/6- 3110/246	-210 329324	3.66
FT/SVWNS DA)	aug-co-pVQZ	-8.76 (-8.70)		MRC(6)+Q/6- 3110(24)	-288-321843	2.54
FT/LDA	26x26x24 cell 100 Rydberg cutoff	-8.88		DFT-B3LYP/6- 311G+(4)	-2.6688843	-9.00
PT/BLYP	20x20x20 cell 70 Rysterg cutoff	-4.33		CCBD(T)wwg- co-pVDZ DFT-PLAP1 XCR-311G+(4)		33
PT/PRE	20x20x20 cell 70 Rydberg cutoff	-6.29				8.18
Lantum Monte Carlo		4.4+0.4	1	Quantum Monte Carlo		-3.4+0.4
speriment		-0.4±0.7	1	Experiment		20:03

- The results presented in this poster are only preliminary ones, more work needs to be done in order using QMC to get better results.

  The QMC results are in fairly agreement with those obtained using other

B. Lichan, A. Strobal, and V. Bonrýbay, J. Chem. Phys. 111, 2020 (192. E. Wade, J. Cline, T. Lonerz, J. Chem. Phys. 116, 4725 (2002). S. Stazzleńsci, S. Coley, W. Kolzu, J. Chem. Phys. 116, 4725 (2002). R. Saryon, R. Valson, J. Arplads, J. Chem. Phys. 12, 6003 (2003). R. Saryon, R. Valson, J. Arplads, J. Chem. Phys. 12, 6003 (2003). M. Pitach, J. Del Barro, J. Birokley, J. Chem. Phys., 84 2279 (1906). J. Geosaman, preprint (2002).